

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.28e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.38e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>17beta-Estradiol</div> <div>Measured: 1.38e-05</div> <div>Predicted: 3.18e-04</div>	<div>Image not found</div> <div>17alpha-Estradiol</div> <div>Measured: 1.38e-05</div> <div>Predicted: 3.18e-04</div>	<div>Image not found</div> <div>Abietic acid</div> <div>Measured: 1.60e-04</div> <div>Predicted: 2.45e-04</div>
<div>Image not found</div> <div>Estrone</div> <div>Measured: 1.11e-04</div> <div>Predicted: 1.91e-04</div>	<div>Image not found</div> <div>Benzyl 4-hydroxyphenyl ketone</div> <div>Measured: 3.16e-02</div> <div>Predicted: 6.55e-03</div>	